Theoretical study of oxygen-evolution reactions by first-principles calculations

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Water electrolysis devices, which can produce hydrogen either directly from solar power or from an external power source, are very attractive as a solution to the growing global demand for energy and the associated environmental problems. However, the slow reaction rate of the oxygen evolution reaction (OER) occurring at the anode of these electrolyzers has hindered the widespread use of such technologies. Therefore, the development of efficient and stable OER catalysts has been actively investigated: IrO_2 is considered the best OER electrocatalysts [1]. The high activity is also known to depend on the surface index, in the following order: $IrO_2(100) > IrO_2(110)$.

In this study, we performed ab initio calculations of the OER catalytic activity of IrO2 with various surface structures and theoretically predicted the order of catalytic activity.

Three density functional methods (PBE, RPBE, and optPBE) implemented in VASP were used to compare the activity of IrO_2 with (110), (100), and (101) surfaces (Fig. 2). The PBE and optPBE results are found consistent with the experimental results [2], but the RPBE one was found to be inconsistent with the expected.
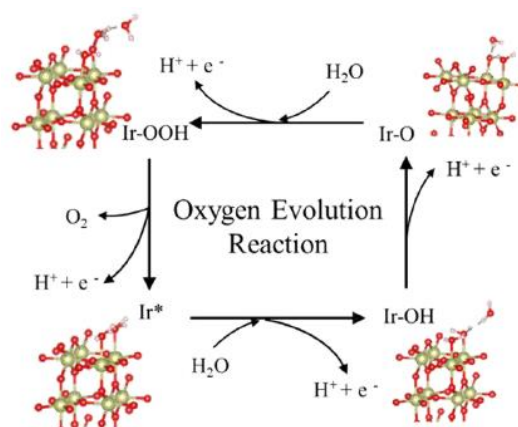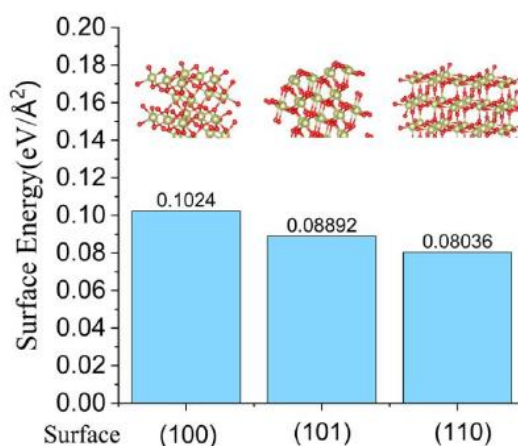

Fig. 1 Mechanism of OER.

Fig. 2 Surface energies of three different surfaces of IrO_2.

References

[1] T. Reier, M. Oezaslan, P. Strasser, ACS Catalysis **2**, 1765 (2012).

[2] L. G. V. Briquet, M. Sarwar, J. Mugo, ChemCatChem **9**, 1261 (2017